wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 08:44 PM EDT

PDB ID	:	2QL3
Title	:	Crystal structure of the C-terminal domain of a probable LysR family transcriptional regulator from Rhodococcus sp. RHA1
Authors	:	Tan, K.; Skarina, T.; Kagen, O.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-07-12
Resolution	:	2.05 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:

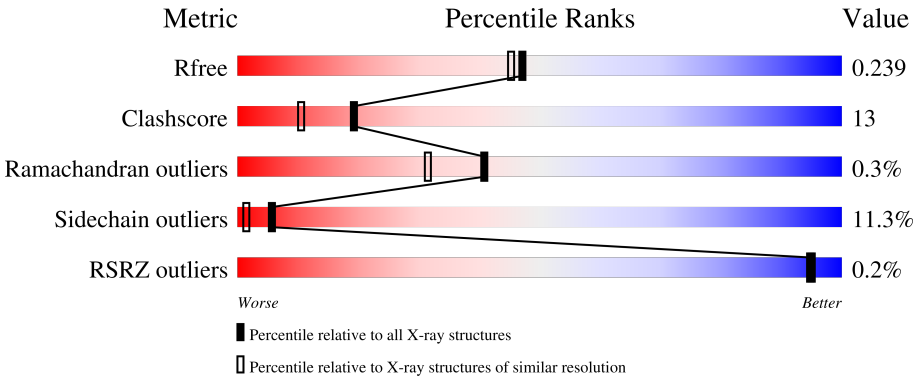
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	209	70% 23%
1	B	209	73% 21%
1	C	209	% 65% 27% 5%
1	D	209	66% 27% 5%
1	E	209	75% 20%

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Mol	Chain	Length	Quality of chain
1	F	209	73% 20% 6%
1	G	209	66% 25% 6%
1	H	209	72% 20% 6%
1	I	209	76% 20%
1	J	209	75% 20%
1	K	209	72% 20% 6%
1	L	209	72% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	1670	-	-	X	-
2	PO4	H	1631	-	-	X	-
2	PO4	K	1669	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20701 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 Probable transcriptional regulator, LysR family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	B	205	Total	C	N	O	S	Se	0	1	0
			1578	1013	274	284	2	5			
1	C	205	Total	C	N	O	S	Se	0	3	0
			1588	1022	274	284	2	6			
1	D	205	Total	C	N	O	S	Se	0	2	0
			1583	1018	274	284	2	5			
1	E	205	Total	C	N	O	S	Se	0	5	0
			1599	1030	277	284	2	6			
1	F	205	Total	C	N	O	S	Se	0	2	0
			1584	1019	274	284	2	5			
1	G	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	H	205	Total	C	N	O	S	Se	0	1	0
			1579	1013	274	284	2	6			
1	I	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	J	205	Total	C	N	O	S	Se	0	1	0
			1578	1013	274	284	2	5			
1	K	205	Total	C	N	O	S	Se	0	1	0
			1579	1013	274	284	2	6			
1	L	205	Total	C	N	O	S	Se	0	1	0
			1582	1015	275	285	2	5			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
A	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
A	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
A	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
A	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
A	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
A	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
B	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
B	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
B	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
B	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
B	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
B	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
B	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
B	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
B	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
C	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
C	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
C	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
C	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
C	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
C	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
C	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
C	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
C	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
D	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
D	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
D	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
D	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
D	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
D	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
D	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
D	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
D	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
E	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
E	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
E	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
E	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
E	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
E	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
E	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
E	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
E	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
F	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
F	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
F	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
F	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
F	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
F	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
F	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
F	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
G	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
G	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
G	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
G	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
G	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
G	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
G	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
G	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
G	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
H	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
H	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
H	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
H	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
H	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
H	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
H	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
H	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
H	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
I	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
I	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
I	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
I	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
I	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
I	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
I	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
I	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
I	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
J	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
J	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
J	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
J	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
J	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
J	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
J	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
J	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8

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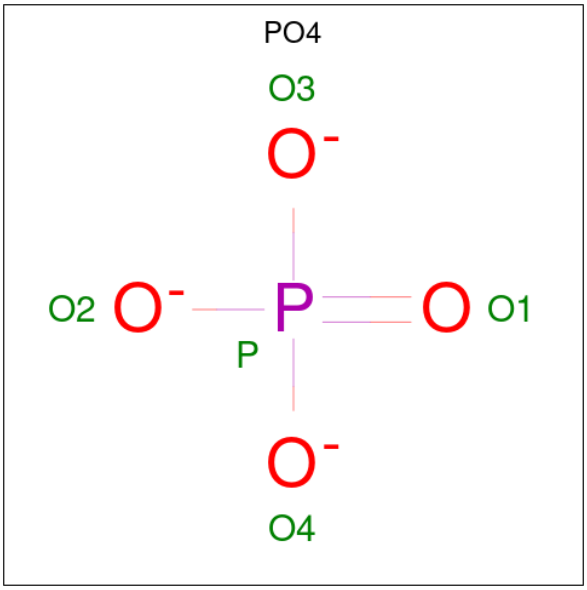
Chain	Residue	Modelled	Actual	Comment	Reference
J	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
K	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
K	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
K	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
K	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
K	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
K	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
K	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
K	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
K	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8
L	97	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
L	98	HIS	-	CLONING ARTIFACT	UNP Q0SFM8
L	119	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
L	171	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
L	176	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
L	202	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
L	215	MSE	MET	MODIFIED RESIDUE	UNP Q0SFM8
L	304	GLY	-	CLONING ARTIFACT	UNP Q0SFM8
L	305	SER	-	CLONING ARTIFACT	UNP Q0SFM8

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



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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	B	118	Total O 118 118	0	0
3	C	67	Total O 67 67	0	0
3	D	90	Total O 90 90	0	0
3	E	122	Total O 122 122	0	0
3	F	109	Total O 109 109	0	0
3	G	81	Total O 81 81	0	0
3	H	93	Total O 93 93	0	0

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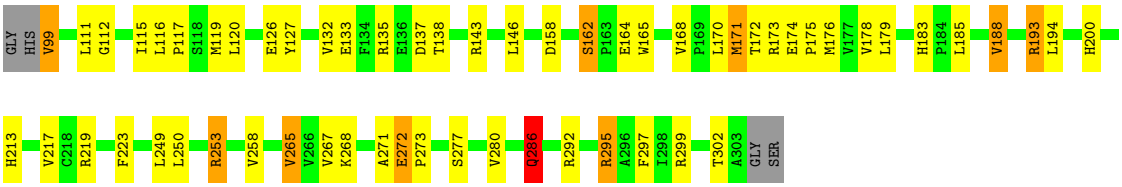
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	135	Total O 135 135	0	0
3	J	130	Total O 130 130	0	0
3	K	121	Total O 121 121	0	0
3	L	167	Total O 167 167	0	0

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.

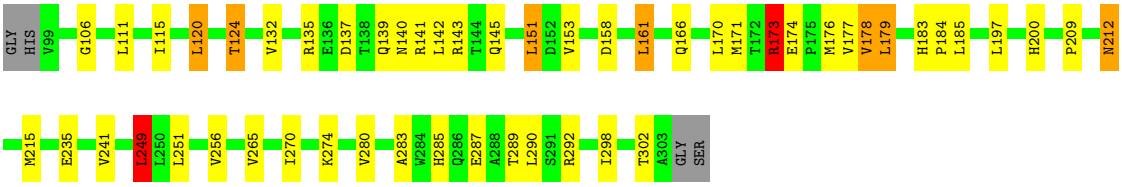
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain A:



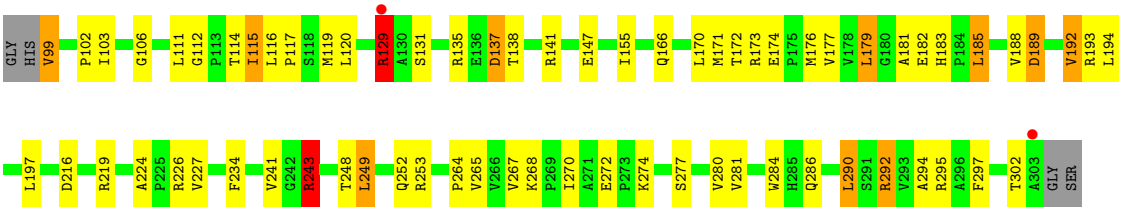
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain B:



• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain C:

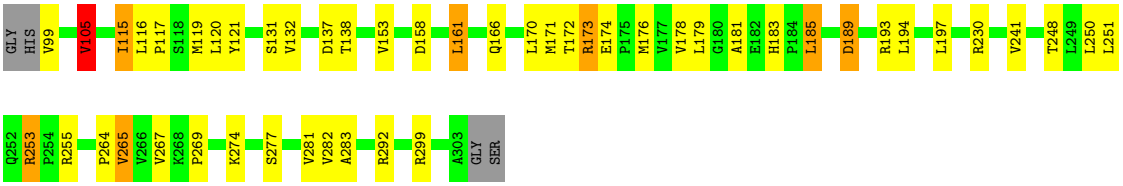


• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain D:

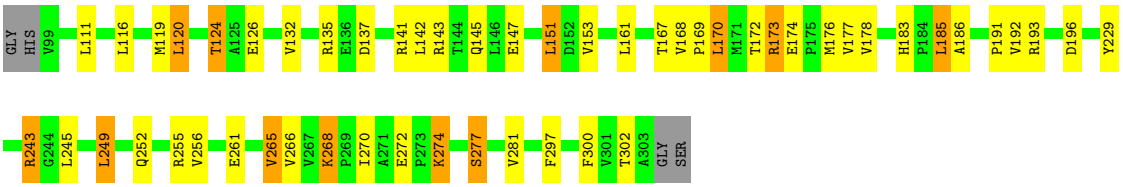
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain E:



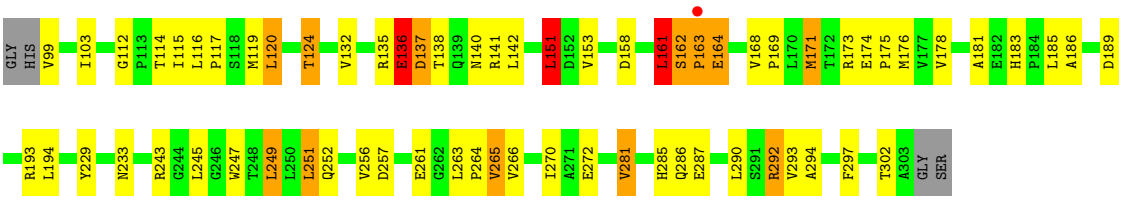
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain F:



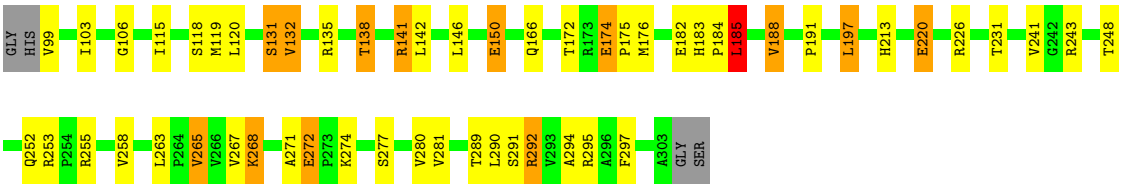
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain G:



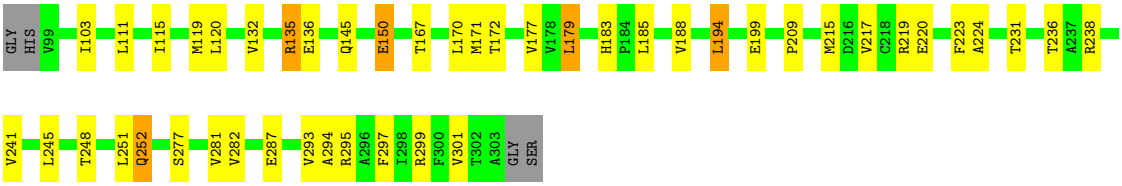
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain H:



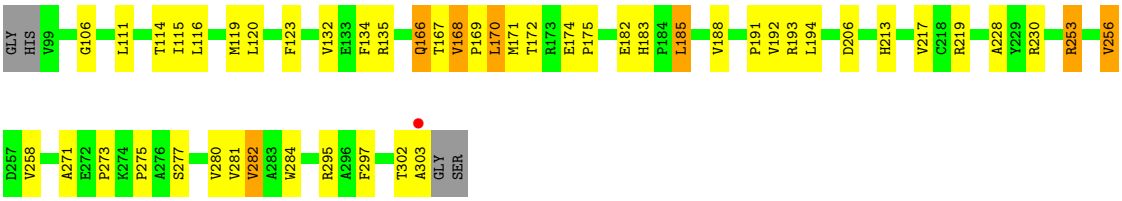
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain I:



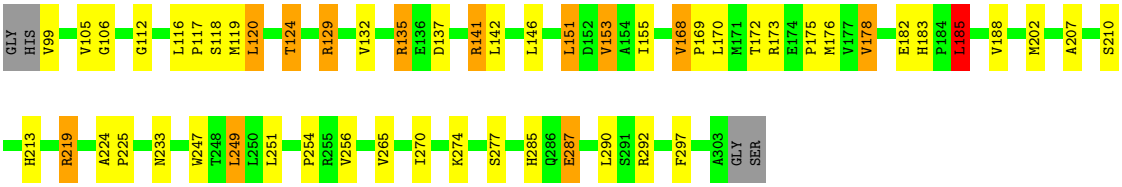
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain J:



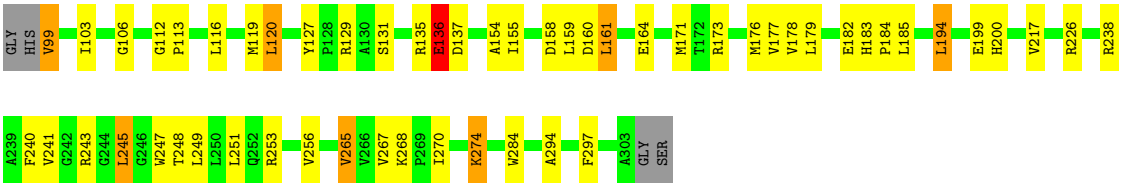
• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain K:



• Molecule 1: Probable transcriptional regulator, LysR family protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	114.28Å 114.28Å 175.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.60 – 2.05 36.58 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.60-2.05) 99.3 (36.58-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.239 0.177 , 0.239	Depositor DCC
R_{free} test set	7989 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.036 for h,-h-k,-l 0.059 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20701	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: 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	0.94	1/1610 (0.1%)	1.00	8/2199 (0.4%)
1	B	0.89	1/1617 (0.1%)	0.98	3/2209 (0.1%)
1	C	0.86	0/1633	0.91	3/2230 (0.1%)
1	D	0.89	0/1625	0.96	2/2220 (0.1%)
1	E	0.96	0/1650	1.02	4/2254 (0.2%)
1	F	0.95	1/1626 (0.1%)	1.01	4/2221 (0.2%)
1	G	0.86	1/1610 (0.1%)	0.93	4/2199 (0.2%)
1	H	0.93	1/1618 (0.1%)	0.94	5/2209 (0.2%)
1	I	1.06	2/1610 (0.1%)	1.04	4/2199 (0.2%)
1	J	0.96	1/1617 (0.1%)	0.96	2/2209 (0.1%)
1	K	0.97	1/1618 (0.1%)	1.03	4/2209 (0.2%)
1	L	1.02	0/1618	1.01	5/2210 (0.2%)
All	All	0.94	9/19452 (0.0%)	0.98	48/26568 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	3
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	136	GLU	CB-CG	-6.16	1.40	1.52
1	H	182	GLU	CB-CG	5.83	1.63	1.52
1	A	126	GLU	CB-CG	5.77	1.63	1.52
1	B	235	GLU	CG-CD	5.76	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	220	GLU	CD-OE2	5.55	1.31	1.25

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	253	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	J	253	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	K	141	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	253	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	F	196	ASP	CB-CG-OD1	-8.01	111.09	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	129	ARG	Peptide
1	G	161	LEU	Peptide
1	G	162	SER	Peptide
1	G	163	PRO	Peptide

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	1574	0	1580	48	0
1	B	1578	0	1589	41	0
1	C	1588	0	1609	47	0
1	D	1583	0	1600	57	0
1	E	1599	0	1629	37	0
1	F	1584	0	1602	38	0
1	G	1574	0	1580	52	0
1	H	1579	0	1589	46	0
1	I	1574	0	1580	31	0
1	J	1578	0	1589	39	0
1	K	1579	0	1589	50	0
1	L	1582	0	1590	35	0
2	A	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	4	0
2	C	30	0	0	3	0
2	D	25	0	0	2	0
2	E	15	0	0	2	0
2	F	70	0	0	3	0
2	G	15	0	0	1	0
2	H	20	0	0	4	0
2	I	35	0	0	0	0
2	J	35	0	0	1	0
2	K	50	0	0	5	0
2	L	30	0	0	1	0
3	A	116	0	0	7	0
3	B	118	0	0	0	0
3	C	67	0	0	1	0
3	D	90	0	0	0	0
3	E	122	0	0	1	0
3	F	109	0	0	3	0
3	G	81	0	0	3	0
3	H	93	0	0	2	0
3	I	135	0	0	7	0
3	J	130	0	0	0	0
3	K	121	0	0	2	0
3	L	167	0	0	2	0
All	All	20701	0	19126	495	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 13.

The worst 5 of 495 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:K:202:MSE:HE2	1:K:247:TRP:CH2	1.75	1.20
1:H:119:MSE:HE3	1:H:297:PHE:HZ	1.18	1.06
1:E:170:LEU:HD11	1:E:282:VAL:CG2	1.87	1.05
1:D:219:ARG:HG2	1:D:219:ARG:HH11	0.88	1.04
1:C:119:MSE:HE3	1:C:297:PHE:HZ	1.21	1.04

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	203/209 (97%)	198 (98%)	3 (2%)	2 (1%)	15 6
1	B	204/209 (98%)	203 (100%)	1 (0%)	0	100 100
1	C	206/209 (99%)	203 (98%)	2 (1%)	1 (0%)	29 18
1	D	205/209 (98%)	198 (97%)	6 (3%)	1 (0%)	29 18
1	E	208/209 (100%)	206 (99%)	2 (1%)	0	100 100
1	F	205/209 (98%)	203 (99%)	2 (1%)	0	100 100
1	G	203/209 (97%)	199 (98%)	3 (2%)	1 (0%)	29 18
1	H	204/209 (98%)	201 (98%)	2 (1%)	1 (0%)	29 18
1	I	203/209 (97%)	199 (98%)	3 (2%)	1 (0%)	29 18
1	J	204/209 (98%)	202 (99%)	2 (1%)	0	100 100
1	K	204/209 (98%)	202 (99%)	2 (1%)	0	100 100
1	L	204/209 (98%)	197 (97%)	6 (3%)	1 (0%)	29 18
All	All	2453/2508 (98%)	2411 (98%)	34 (1%)	8 (0%)	41 31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	VAL
1	A	188	VAL
1	G	164	GLU
1	I	188	VAL
1	A	286	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	165/162 (102%)	148 (90%)	17 (10%)	7 2
1	B	166/162 (102%)	147 (89%)	19 (11%)	5 1
1	C	168/162 (104%)	145 (86%)	23 (14%)	3 1
1	D	167/162 (103%)	148 (89%)	19 (11%)	5 1
1	E	170/162 (105%)	152 (89%)	18 (11%)	6 2
1	F	167/162 (103%)	148 (89%)	19 (11%)	5 1
1	G	165/162 (102%)	141 (86%)	24 (14%)	3 1
1	H	166/162 (102%)	146 (88%)	20 (12%)	5 1
1	I	165/162 (102%)	150 (91%)	15 (9%)	9 3
1	J	166/162 (102%)	152 (92%)	14 (8%)	11 4
1	K	166/162 (102%)	146 (88%)	20 (12%)	5 1
1	L	166/162 (102%)	147 (89%)	19 (11%)	5 1
All	All	1997/1944 (103%)	1770 (89%)	227 (11%)	6 1

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	120	LEU
1	L	194	LEU
1	H	146	LEU
1	L	179	LEU
1	K	176[B]	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	183	HIS
1	L	183	HIS
1	J	183	HIS
1	K	213	HIS
1	D	183	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

76 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	C	1607	-	4,4,4	0.66	0	6,6,6	1.16	1 (16%)
2	PO4	A	1616	-	4,4,4	0.88	0	6,6,6	0.55	0
2	PO4	F	1639	-	4,4,4	0.93	0	6,6,6	0.63	0
2	PO4	C	1612	-	4,4,4	1.02	0	6,6,6	0.32	0
2	PO4	K	1620	-	4,4,4	0.33	0	6,6,6	1.27	0
2	PO4	F	1627	-	4,4,4	0.71	0	6,6,6	0.76	0
2	PO4	H	1617	-	4,4,4	0.90	0	6,6,6	0.82	0
2	PO4	H	1604	-	4,4,4	0.99	0	6,6,6	1.19	1 (16%)
2	PO4	I	1606	-	4,4,4	1.04	0	6,6,6	1.38	1 (16%)
2	PO4	J	1667	-	4,4,4	0.87	0	6,6,6	0.72	0
2	PO4	L	1622	-	4,4,4	1.12	0	6,6,6	1.08	1 (16%)
2	PO4	A	1641	-	4,4,4	0.91	0	6,6,6	1.13	1 (16%)
2	PO4	I	1655	-	4,4,4	0.55	0	6,6,6	1.34	1 (16%)
2	PO4	A	1615	-	4,4,4	0.90	0	6,6,6	0.61	0
2	PO4	B	1670	-	4,4,4	0.89	0	6,6,6	0.71	0
2	PO4	C	1623	-	4,4,4	1.01	0	6,6,6	0.60	0
2	PO4	K	1610	-	4,4,4	0.88	0	6,6,6	0.65	0
2	PO4	D	1629	-	4,4,4	0.88	0	6,6,6	0.77	0
2	PO4	G	1678	-	4,4,4	1.10	0	6,6,6	0.74	0
2	PO4	J	1633	-	4,4,4	0.69	0	6,6,6	0.87	0
2	PO4	A	1664	-	4,4,4	0.72	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	I	1665	-	4,4,4	0.96	0	6,6,6	0.33	0
2	PO4	K	1601	-	4,4,4	0.83	0	6,6,6	1.59	1 (16%)
2	PO4	F	1611	-	4,4,4	0.59	0	6,6,6	1.15	0
2	PO4	H	1676	-	4,4,4	0.68	0	6,6,6	0.89	0
2	PO4	J	1653	-	4,4,4	0.64	0	6,6,6	0.57	0
2	PO4	I	1662	-	4,4,4	0.79	0	6,6,6	0.79	0
2	PO4	K	1669	-	4,4,4	0.82	0	6,6,6	0.71	0
2	PO4	G	1637	-	4,4,4	0.54	0	6,6,6	1.14	1 (16%)
2	PO4	F	1605	-	4,4,4	0.95	0	6,6,6	0.87	0
2	PO4	H	1631	-	4,4,4	0.89	0	6,6,6	0.55	0
2	PO4	B	1638	-	4,4,4	1.02	0	6,6,6	0.59	0
2	PO4	B	1630	-	4,4,4	1.00	0	6,6,6	0.86	0
2	PO4	F	1618	-	4,4,4	0.87	0	6,6,6	0.71	0
2	PO4	I	1632	-	4,4,4	0.83	0	6,6,6	1.04	0
2	PO4	K	1672	-	4,4,4	0.73	0	6,6,6	0.93	0
2	PO4	E	1624	-	4,4,4	0.97	0	6,6,6	0.31	0
2	PO4	I	1621	-	4,4,4	0.85	0	6,6,6	1.39	1 (16%)
2	PO4	K	1673	-	4,4,4	1.04	0	6,6,6	1.07	0
2	PO4	L	1609	-	4,4,4	0.90	0	6,6,6	0.65	0
2	PO4	I	1645	-	4,4,4	0.70	0	6,6,6	0.83	0
2	PO4	F	1647	-	4,4,4	0.84	0	6,6,6	0.69	0
2	PO4	D	1660	-	4,4,4	0.98	0	6,6,6	0.65	0
2	PO4	F	1646	-	4,4,4	0.65	0	6,6,6	0.73	0
2	PO4	K	1608	-	4,4,4	0.98	0	6,6,6	0.52	0
2	PO4	F	1652	-	4,4,4	0.88	0	6,6,6	0.60	0
2	PO4	D	1659	-	4,4,4	0.79	0	6,6,6	0.77	0
2	PO4	F	1640	-	4,4,4	0.82	0	6,6,6	0.51	0
2	PO4	A	1674	-	4,4,4	0.94	0	6,6,6	0.71	0
2	PO4	C	1619	-	4,4,4	0.83	0	6,6,6	1.59	1 (16%)
2	PO4	E	1642	-	4,4,4	0.90	0	6,6,6	0.48	0
2	PO4	B	1651	-	4,4,4	0.97	0	6,6,6	0.75	0
2	PO4	J	1614	-	4,4,4	0.72	0	6,6,6	0.51	0
2	PO4	F	1636	-	4,4,4	0.85	0	6,6,6	0.71	0
2	PO4	J	1603	-	4,4,4	0.62	0	6,6,6	0.87	0
2	PO4	F	1650	-	4,4,4	0.89	0	6,6,6	0.58	0
2	PO4	K	1661	-	4,4,4	0.82	0	6,6,6	0.75	0
2	PO4	A	1626	-	4,4,4	0.95	0	6,6,6	0.93	0
2	PO4	E	1644	-	4,4,4	0.94	0	6,6,6	0.69	0
2	PO4	C	1648	-	4,4,4	0.87	0	6,6,6	0.66	0
2	PO4	L	1656	-	4,4,4	0.44	0	6,6,6	1.41	1 (16%)
2	PO4	B	1677	-	4,4,4	0.69	0	6,6,6	0.88	0
2	PO4	J	1613	-	4,4,4	0.95	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	J	1668	-	4,4,4	0.73	0	6,6,6	0.75	0
2	PO4	L	1602	-	4,4,4	1.29	0	6,6,6	1.51	1 (16%)
2	PO4	L	1643	-	4,4,4	0.83	0	6,6,6	0.65	0
2	PO4	K	1625	-	4,4,4	0.83	0	6,6,6	0.43	0
2	PO4	K	1634	-	4,4,4	0.91	0	6,6,6	0.63	0
2	PO4	L	1666	-	4,4,4	0.86	0	6,6,6	0.59	0
2	PO4	D	1658	-	4,4,4	0.98	0	6,6,6	0.80	0
2	PO4	D	1657	-	4,4,4	0.84	0	6,6,6	0.71	0
2	PO4	F	1675	-	4,4,4	0.50	0	6,6,6	0.82	0
2	PO4	G	1654	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	C	1663	-	4,4,4	0.72	0	6,6,6	0.59	0
2	PO4	F	1628	-	4,4,4	1.07	0	6,6,6	1.10	1 (16%)
2	PO4	F	1635	-	4,4,4	0.46	0	6,6,6	0.62	0

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1619	PO4	O4-P-O2	3.06	117.44	107.91
2	L	1602	PO4	O3-P-O2	2.78	116.57	107.91
2	I	1621	PO4	O2-P-O1	-2.63	101.64	110.95
2	H	1604	PO4	O4-P-O3	2.63	116.10	107.91
2	L	1656	PO4	O2-P-O1	-2.63	101.66	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1607	PO4	1	0
2	K	1620	PO4	1	0
2	H	1617	PO4	1	0
2	B	1670	PO4	3	0
2	G	1678	PO4	1	0
2	K	1669	PO4	2	0
2	H	1631	PO4	3	0
2	E	1624	PO4	1	0
2	K	1673	PO4	1	0
2	D	1660	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1608	PO4	1	0
2	A	1674	PO4	1	0
2	C	1619	PO4	1	0
2	B	1651	PO4	1	0
2	F	1650	PO4	1	0
2	A	1626	PO4	1	0
2	E	1644	PO4	1	0
2	L	1656	PO4	1	0
2	J	1668	PO4	1	0
2	D	1657	PO4	1	0
2	F	1675	PO4	1	0
2	C	1663	PO4	1	0
2	F	1628	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	200/209 (95%)	-0.41	0 100 100	23, 30, 39, 44	0
1	B	200/209 (95%)	-0.30	0 100 100	23, 32, 46, 49	0
1	C	200/209 (95%)	-0.10	2 (1%) 82 84	26, 36, 47, 53	0
1	D	200/209 (95%)	-0.27	0 100 100	26, 33, 44, 52	0
1	E	200/209 (95%)	-0.42	0 100 100	22, 29, 41, 49	0
1	F	200/209 (95%)	-0.40	0 100 100	21, 30, 40, 45	0
1	G	200/209 (95%)	-0.08	1 (0%) 91 92	25, 37, 53, 58	0
1	H	200/209 (95%)	-0.28	0 100 100	22, 32, 45, 51	0
1	I	200/209 (95%)	-0.44	0 100 100	20, 26, 38, 46	0
1	J	200/209 (95%)	-0.35	1 (0%) 91 92	21, 29, 40, 48	0
1	K	200/209 (95%)	-0.34	0 100 100	21, 29, 42, 47	0
1	L	200/209 (95%)	-0.41	0 100 100	20, 27, 38, 50	0
All	All	2400/2508 (95%)	-0.32	4 (0%) 95 95	20, 31, 45, 58	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	163	PRO	3.3
1	C	303	ALA	3.2
1	C	129	ARG	2.6
1	J	303	ALA	2.1

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

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
2	PO4	B	1677	5/5	0.52	0.36	88,89,90,91	0
2	PO4	A	1641	5/5	0.68	0.33	67,67,70,74	0
2	PO4	L	1622	5/5	0.69	0.28	77,79,81,81	0
2	PO4	L	1643	5/5	0.70	0.20	113,113,114,114	0
2	PO4	F	1652	5/5	0.75	0.33	128,128,128,128	0
2	PO4	L	1656	5/5	0.75	0.30	71,75,77,77	0
2	PO4	F	1640	5/5	0.78	0.25	92,92,93,94	0
2	PO4	J	1653	5/5	0.79	0.26	112,112,113,113	0
2	PO4	B	1651	5/5	0.79	0.22	91,92,93,94	0
2	PO4	H	1676	5/5	0.80	0.22	81,81,83,83	0
2	PO4	J	1633	5/5	0.80	0.20	90,91,91,92	0
2	PO4	G	1654	5/5	0.80	0.19	134,135,135,135	0
2	PO4	I	1655	5/5	0.81	0.32	66,68,70,73	0
2	PO4	E	1642	5/5	0.82	0.17	104,104,105,106	0
2	PO4	F	1618	5/5	0.82	0.27	86,87,88,88	0
2	PO4	F	1650	5/5	0.83	0.39	96,96,97,97	0
2	PO4	F	1639	5/5	0.83	0.21	91,91,92,92	0
2	PO4	F	1611	5/5	0.85	0.14	64,65,67,68	0
2	PO4	D	1660	5/5	0.85	0.21	66,67,70,70	0
2	PO4	E	1624	5/5	0.86	0.16	92,93,93,94	0
2	PO4	D	1629	5/5	0.86	0.17	67,68,72,72	0
2	PO4	F	1675	5/5	0.87	0.21	75,76,78,78	0
2	PO4	D	1657	5/5	0.88	0.20	93,94,94,94	0
2	PO4	A	1674	5/5	0.89	0.25	78,78,79,79	0
2	PO4	C	1663	5/5	0.89	0.36	93,93,94,94	0
2	PO4	I	1662	5/5	0.89	0.20	66,69,69,70	0
2	PO4	A	1664	5/5	0.89	0.18	91,91,92,92	0
2	PO4	G	1637	5/5	0.90	0.18	65,66,69,69	0
2	PO4	F	1646	5/5	0.90	0.15	75,76,78,78	0
2	PO4	J	1667	5/5	0.90	0.24	92,92,93,93	0
2	PO4	K	1673	5/5	0.90	0.20	68,68,71,71	0
2	PO4	B	1638	5/5	0.90	0.18	76,78,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	C	1623	5/5	0.90	0.16	77,78,79,80	0
2	PO4	A	1616	5/5	0.90	0.24	72,72,74,74	0
2	PO4	A	1615	5/5	0.91	0.20	71,71,72,73	0
2	PO4	E	1644	5/5	0.91	0.17	68,68,70,70	0
2	PO4	K	1620	5/5	0.92	0.18	55,58,58,60	0
2	PO4	K	1625	5/5	0.92	0.19	88,88,89,89	0
2	PO4	K	1669	5/5	0.92	0.17	81,82,82,83	0
2	PO4	K	1672	5/5	0.92	0.21	59,61,62,64	0
2	PO4	I	1632	5/5	0.92	0.27	77,78,79,80	0
2	PO4	D	1659	5/5	0.92	0.14	76,76,77,77	0
2	PO4	C	1648	5/5	0.92	0.17	85,85,86,87	0
2	PO4	K	1608	5/5	0.92	0.12	83,83,83,84	0
2	PO4	H	1631	5/5	0.93	0.15	61,64,66,66	0
2	PO4	G	1678	5/5	0.93	0.32	45,46,47,51	0
2	PO4	I	1606	5/5	0.93	0.11	46,49,53,56	0
2	PO4	K	1610	5/5	0.93	0.11	61,63,64,65	0
2	PO4	J	1613	5/5	0.93	0.12	69,70,71,73	0
2	PO4	I	1621	5/5	0.93	0.12	60,60,61,64	0
2	PO4	F	1647	5/5	0.94	0.20	77,77,78,78	0
2	PO4	I	1665	5/5	0.94	0.09	90,90,90,90	0
2	PO4	K	1634	5/5	0.94	0.18	91,92,92,93	0
2	PO4	J	1614	5/5	0.95	0.11	59,60,61,62	0
2	PO4	D	1658	5/5	0.95	0.40	45,46,47,48	0
2	PO4	I	1645	5/5	0.95	0.14	64,66,67,67	0
2	PO4	L	1609	5/5	0.95	0.17	54,56,59,59	0
2	PO4	F	1636	5/5	0.95	0.23	54,55,57,58	0
2	PO4	J	1668	5/5	0.95	0.28	78,78,79,80	0
2	PO4	K	1661	5/5	0.95	0.29	90,90,90,90	0
2	PO4	L	1666	5/5	0.95	0.24	86,86,86,87	0
2	PO4	H	1617	5/5	0.96	0.17	55,56,57,58	0
2	PO4	F	1635	5/5	0.96	0.13	46,47,51,53	0
2	PO4	A	1626	5/5	0.96	0.12	27,34,41,42	0
2	PO4	C	1619	5/5	0.96	0.17	49,49,51,53	0
2	PO4	B	1670	5/5	0.96	0.22	71,73,74,74	0
2	PO4	H	1604	5/5	0.96	0.12	53,54,56,56	0
2	PO4	F	1628	5/5	0.97	0.11	54,54,57,58	0
2	PO4	C	1607	5/5	0.98	0.12	34,42,45,45	0
2	PO4	J	1603	5/5	0.98	0.14	36,38,39,42	0
2	PO4	C	1612	5/5	0.98	0.08	62,62,63,63	0
2	PO4	K	1601	5/5	0.98	0.07	29,29,32,33	0
2	PO4	F	1605	5/5	0.98	0.12	47,49,51,52	0
2	PO4	B	1630	5/5	0.98	0.25	58,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	L	1602	5/5	0.99	0.07	44,45,46,48	0
2	PO4	F	1627	5/5	0.99	0.05	46,47,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.