wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 02:59 AM EDT

PDB ID	:	1RZR
Title	:	crystal structure of transcriptional regulator-phosphoprotein-DNA complex
Authors	:	Schumacher, M.A.; Allen, G.S.; Brennan, R.G.
Deposited on	:	2003-12-27
Resolution	:	2.80 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 (1)) were used in the production of this report:

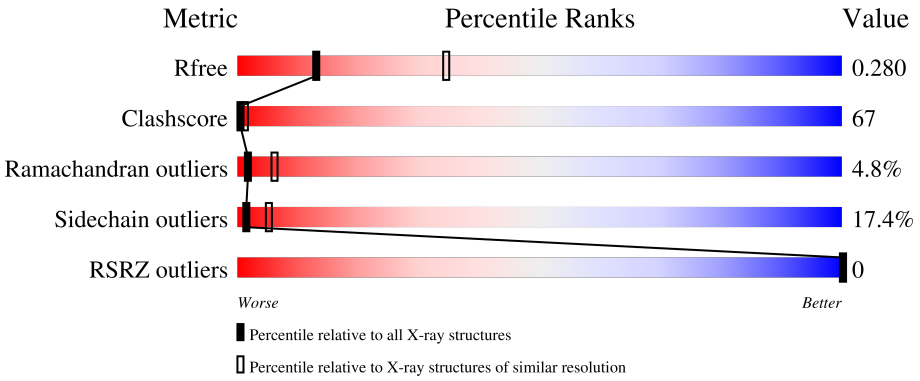
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	E	16	88% 12%
1	H	16	88% 12%
2	B	16	75% 25%
2	R	16	6% 81% 12%
3	A	332	24% 60% 15% .

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Mol	Chain	Length	Quality of chain
3	C	332	24% 60% 15%
3	G	332	29% 53% 17%
4	D	332	24% 60% 16%
5	L	88	32% 55% 13%
5	S	88	28% 58% 13%
5	T	88	31% 49% 19%
5	Y	88	40% 41% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SEP	Y	46	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14194 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 DNA chain called 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			
1	E	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			
2	B	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			

- Molecule 3 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	332	Total	C	N	O	Se	0	0	0
			2564	1610	438	506	10			
3	C	332	Total	C	N	O	Se	0	0	0
			2558	1606	437	505	10			
3	A	332	Total	C	N	O	Se	0	0	0
			2562	1608	437	507	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P46828
A	16	MSE	MET	modified residue	UNP P46828
A	88	MSE	MET	modified residue	UNP P46828
A	112	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
A	123	MSE	MET	modified residue	UNP P46828
A	250	MSE	MET	modified residue	UNP P46828
A	282	MSE	MET	modified residue	UNP P46828
A	294	MSE	MET	modified residue	UNP P46828
A	302	MSE	MET	modified residue	UNP P46828
A	309	MSE	MET	modified residue	UNP P46828
C	1	MSE	MET	modified residue	UNP P46828
C	16	MSE	MET	modified residue	UNP P46828
C	88	MSE	MET	modified residue	UNP P46828
C	112	MSE	MET	modified residue	UNP P46828
C	123	MSE	MET	modified residue	UNP P46828
C	250	MSE	MET	modified residue	UNP P46828
C	282	MSE	MET	modified residue	UNP P46828
C	294	MSE	MET	modified residue	UNP P46828
C	302	MSE	MET	modified residue	UNP P46828
C	309	MSE	MET	modified residue	UNP P46828
G	1	MSE	MET	modified residue	UNP P46828
G	16	MSE	MET	modified residue	UNP P46828
G	88	MSE	MET	modified residue	UNP P46828
G	112	MSE	MET	modified residue	UNP P46828
G	123	MSE	MET	modified residue	UNP P46828
G	250	MSE	MET	modified residue	UNP P46828
G	282	MSE	MET	modified residue	UNP P46828
G	294	MSE	MET	modified residue	UNP P46828
G	302	MSE	MET	modified residue	UNP P46828
G	309	MSE	MET	modified residue	UNP P46828

- Molecule 4 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	332	Total	C	N	O	S	Se	0	0	0
			2558	1606	437	505	1	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	16	MSE	MET	modified residue	UNP P46828
D	88	MSE	MET	modified residue	UNP P46828
D	112	MSE	MET	modified residue	UNP P46828
D	123	MSE	MET	modified residue	UNP P46828
D	250	MSE	MET	modified residue	UNP P46828
D	282	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	MSE	MET	modified residue	UNP P46828
D	302	MSE	MET	modified residue	UNP P46828
D	309	MSE	MET	modified residue	UNP P46828

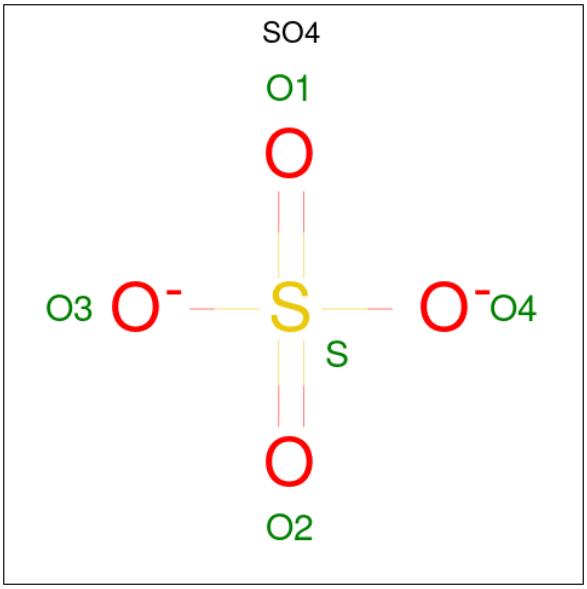
- Molecule 5 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	T	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	L	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	Y	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	S	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	46	SEP	SER	modified residue	UNP O69250
T	46	SEP	SER	modified residue	UNP O69250
L	46	SEP	SER	modified residue	UNP O69250
Y	46	SEP	SER	modified residue	UNP O69250

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total O 1 1	0	0
8	R	1	Total O 1 1	0	0
8	E	2	Total O 2 2	0	0
8	B	1	Total O 1 1	0	0
8	G	10	Total O 10 10	0	0
8	C	13	Total O 13 13	0	0
8	A	17	Total O 17 17	0	0
8	D	12	Total O 12 12	0	0
8	T	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	4	Total O 4 4	0	0
8	Y	10	Total O 10 10	0	0
8	S	7	Total O 7 7	0	0

3 Residue-property plots (i)

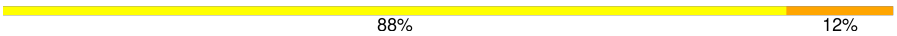
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'

Chain H:

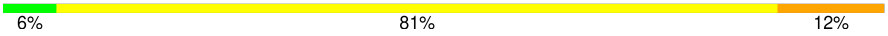
• Molecule 1: 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'

Chain E:



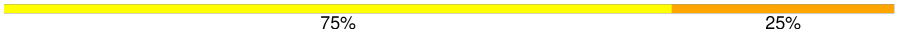
• Molecule 2: 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'

Chain R:



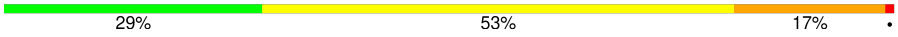
• Molecule 2: 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'

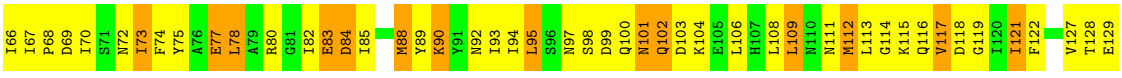
Chain B:

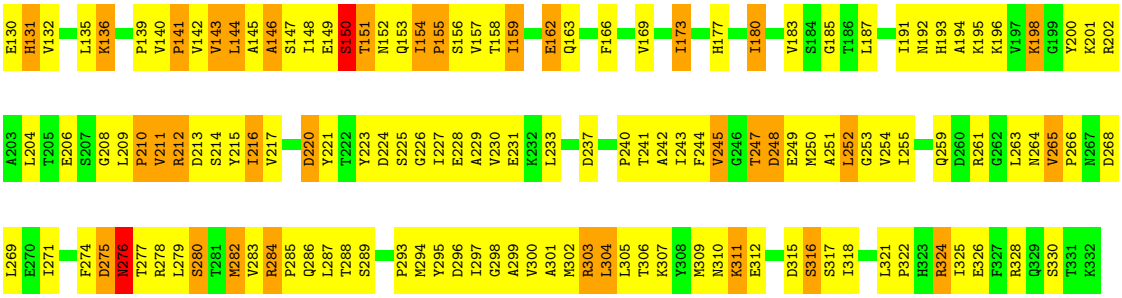


• Molecule 3: Glucose-resistance amylase regulator

Chain G:

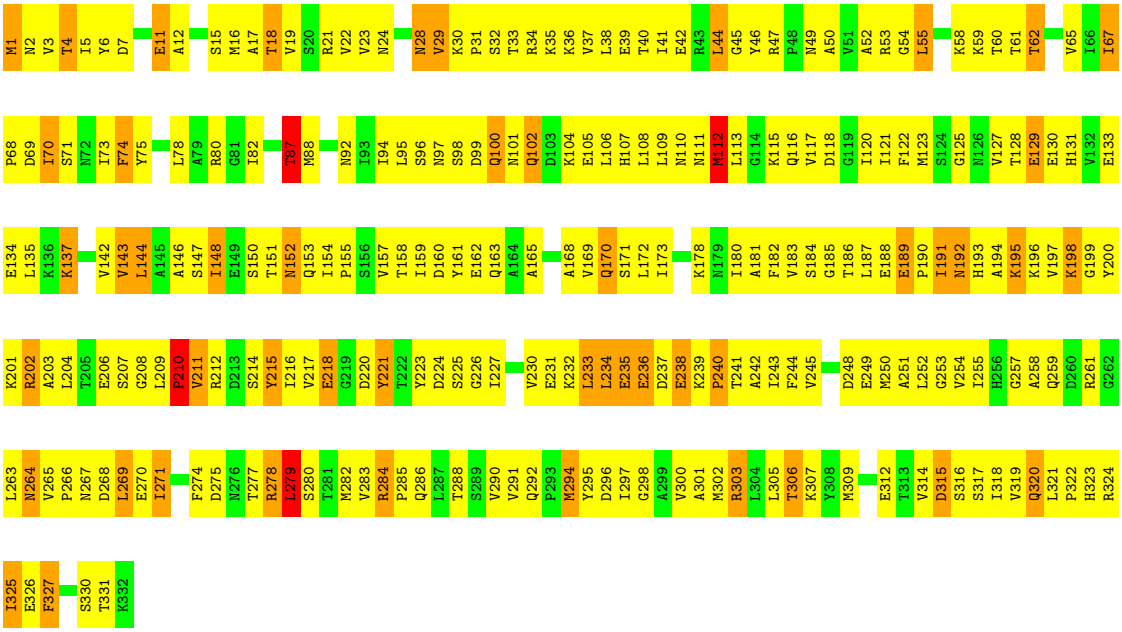






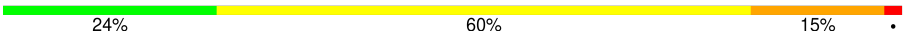
• Molecule 3: Glucose-resistance amylase regulator

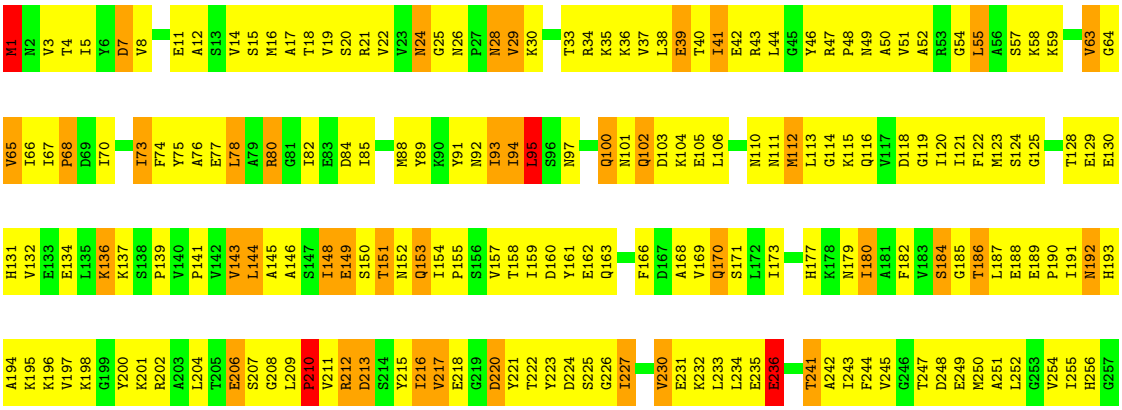
Chain C:

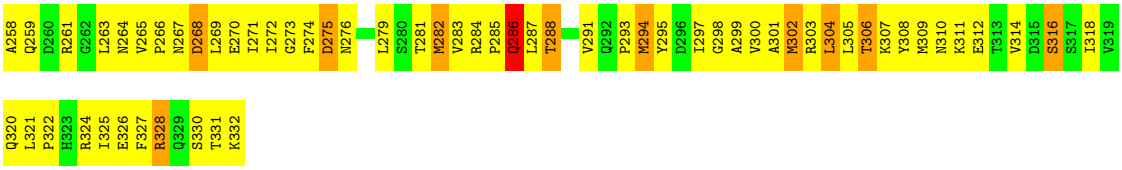


• Molecule 3: Glucose-resistance amylase regulator

Chain A:

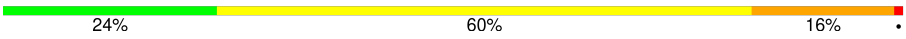


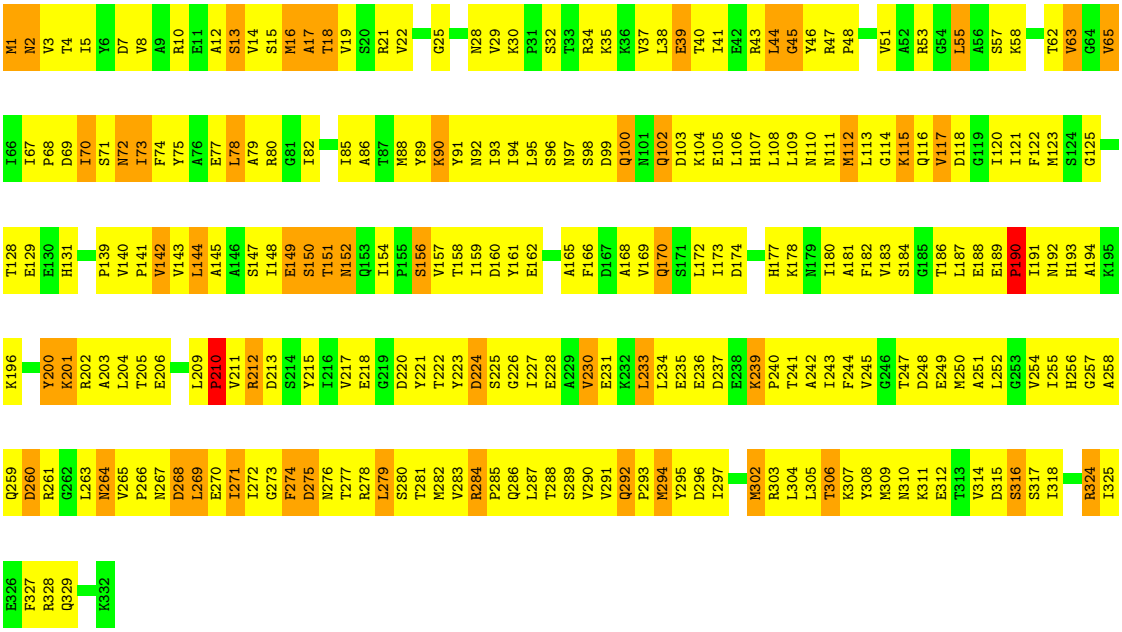




• Molecule 4: Glucose-resistance amylase regulator

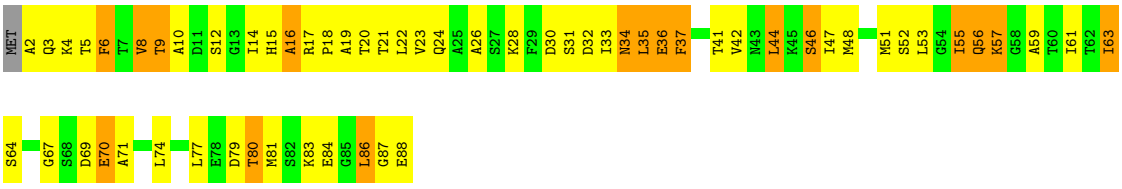
Chain D:





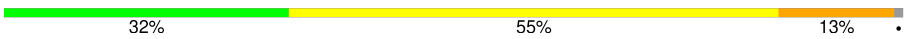
• Molecule 5: Phosphocarrier protein HPr

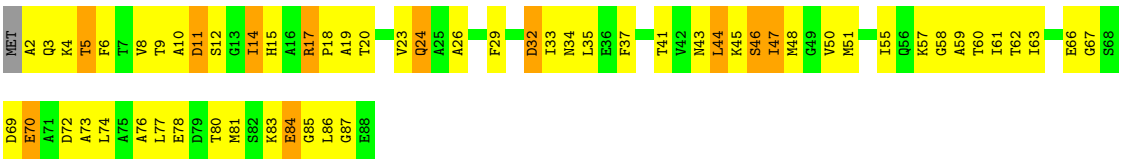
Chain T:



• Molecule 5: Phosphocarrier protein HPr

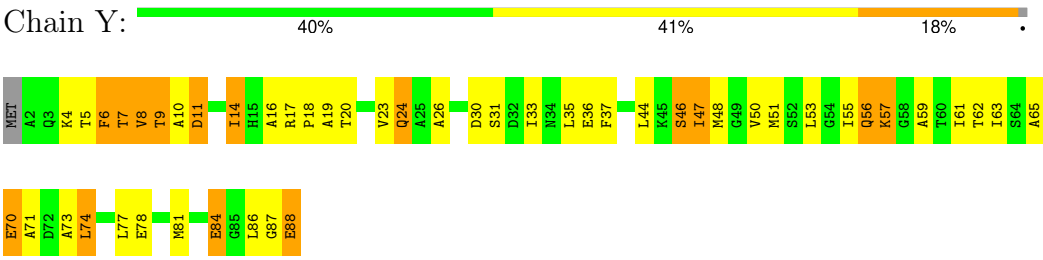
Chain L:





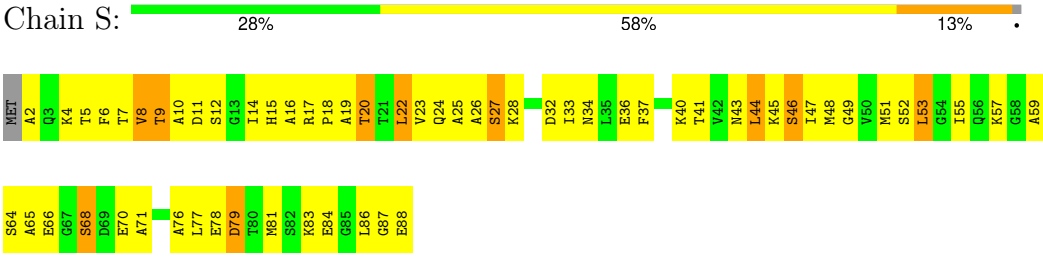
• Molecule 5: Phosphocarrier protein HPr

Chain Y:



• Molecule 5: Phosphocarrier protein HPr

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.71Å 109.24Å 117.81Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	78.70 – 2.80 78.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (78.70-2.80) 86.7 (78.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.288 0.234 , 0.280	Depositor DCC
R_{free} test set	5845 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 107.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l 0.038 for k,h,-l 0.349 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14194	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: SO4, MG, SEP

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	E	0.75	0/368	0.89	0/566
1	H	1.03	3/368 (0.8%)	0.94	1/566 (0.2%)
2	B	0.70	0/360	0.95	0/554
2	R	0.74	0/360	1.00	0/554
3	A	0.73	7/2590 (0.3%)	0.85	3/3492 (0.1%)
3	C	0.68	3/2586 (0.1%)	0.85	3/3486 (0.1%)
3	G	0.73	4/2593 (0.2%)	0.93	8/3498 (0.2%)
4	D	0.66	3/2586 (0.1%)	0.83	1/3486 (0.0%)
5	L	0.51	0/625	0.75	0/839
5	S	0.54	0/625	0.76	0/839
5	T	0.53	0/625	0.75	0/839
5	Y	0.56	0/625	0.87	1/839 (0.1%)
All	All	0.69	20/14311 (0.1%)	0.86	17/19558 (0.1%)

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	E	0	2
1	H	0	1
2	B	0	4
2	R	0	2
4	D	0	1
5	Y	0	1
All	All	0	11

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	MSE	SE-CE	11.43	2.62	1.95
3	A	129	GLU	CD-OE1	9.85	1.36	1.25
4	D	129	GLU	CD-OE1	9.60	1.36	1.25
3	C	129	GLU	CD-OE1	8.89	1.35	1.25
3	C	129	GLU	CD-OE2	8.75	1.35	1.25

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	711	DA	C8-N9-C4	-9.02	102.19	105.80
3	A	236	GLU	N-CA-C	-7.22	91.49	111.00
3	A	95	LEU	CA-CB-CG	6.44	130.10	115.30
3	G	3	VAL	N-CA-C	6.43	128.36	111.00
3	C	1	MSE	CB-CG-SE	-6.39	93.53	112.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	702	DG	Sidechain
1	E	703	DA	Sidechain
1	H	700	DC	Sidechain
2	R	712	DT	Sidechain
2	R	715	DG	Sidechain

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	E	327	0	180	52	0
1	H	327	0	180	56	0
2	B	323	0	184	43	0
2	R	323	0	184	57	0
3	A	2562	0	2587	389	0
3	C	2558	0	2584	386	1
3	G	2564	0	2594	374	1
4	D	2558	0	2584	376	0
5	L	632	0	624	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	632	0	624	69	0
5	T	632	0	624	79	0
5	Y	632	0	624	69	0
6	A	10	0	0	1	0
6	C	15	0	0	1	0
6	G	10	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	17	0	0	0	0
8	B	1	0	0	0	0
8	C	13	0	0	0	0
8	D	12	0	0	0	0
8	E	2	0	0	0	0
8	G	10	0	0	0	0
8	H	1	0	0	0	0
8	L	4	0	0	0	0
8	R	1	0	0	0	0
8	S	7	0	0	0	0
8	T	9	0	0	0	0
8	Y	10	0	0	0	0
All	All	14194	0	13573	1861	1

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 67.

The worst 5 of 1861 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)
3:C:1:MSE:CE	3:C:1:MSE:SE	2.20	1.40
4:D:1:MET:CE	4:D:1:MET:SD	2.15	1.34
3:G:139:PRO:CG	3:C:1:MSE:HE2	1.66	1.26
3:G:73:ILE:CG2	3:C:278:ARG:HH22	1.53	1.22
3:G:73:ILE:HG22	3:C:278:ARG:NH2	1.54	1.21

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:LYS:NZ	3:C:133:GLU:OE1[2_556]	2.17	0.03

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
3	A	330/332 (99%)	259 (78%)	56 (17%)	15 (4%)	2 7
3	C	330/332 (99%)	251 (76%)	62 (19%)	17 (5%)	1 5
3	G	330/332 (99%)	271 (82%)	40 (12%)	19 (6%)	1 4
4	D	330/332 (99%)	246 (74%)	63 (19%)	21 (6%)	1 3
5	L	84/88 (96%)	71 (84%)	12 (14%)	1 (1%)	11 34
5	S	84/88 (96%)	76 (90%)	7 (8%)	1 (1%)	11 34
5	T	84/88 (96%)	72 (86%)	8 (10%)	4 (5%)	2 6
5	Y	84/88 (96%)	73 (87%)	10 (12%)	1 (1%)	11 34
All	All	1656/1680 (99%)	1319 (80%)	258 (16%)	79 (5%)	2 6

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	100	GLN
3	G	102	GLN
3	G	141	PRO
3	G	150	SER
3	G	151	THR

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
3	A	286/279 (102%)	240 (84%)	46 (16%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	285/279 (102%)	241 (85%)	44 (15%)	2 7
3	G	287/279 (103%)	235 (82%)	52 (18%)	1 4
4	D	285/280 (102%)	236 (83%)	49 (17%)	1 5
5	L	66/67 (98%)	54 (82%)	12 (18%)	1 4
5	S	66/67 (98%)	53 (80%)	13 (20%)	1 3
5	T	66/67 (98%)	51 (77%)	15 (23%)	0 2
5	Y	66/67 (98%)	52 (79%)	14 (21%)	1 3
All	All	1407/1385 (102%)	1162 (83%)	245 (17%)	1 5

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	148	ILE
5	Y	11	ASP
4	D	13	SER
5	Y	8	VAL
5	S	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	72	ASN
4	D	267	ASN
4	D	97	ASN
4	D	170	GLN
5	T	3	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
5	SEP	T	46	5	8,9,10	1.20	1 (12%)	7,12,14	1.46	2 (28%)
5	SEP	Y	46	5	8,9,10	1.21	1 (12%)	7,12,14	1.26	1 (14%)
5	SEP	S	46	5	8,9,10	1.17	1 (12%)	7,12,14	1.67	2 (28%)
5	SEP	L	46	5	8,9,10	1.21	1 (12%)	7,12,14	1.32	1 (14%)

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
5	SEP	T	46	5	-	5/6/8/10	-
5	SEP	Y	46	5	-	3/6/8/10	-
5	SEP	S	46	5	-	6/6/8/10	-
5	SEP	L	46	5	-	4/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	46	SEP	P-O3P	-2.56	1.45	1.54
5	L	46	SEP	P-O3P	-2.49	1.45	1.54
5	Y	46	SEP	P-O3P	-2.43	1.45	1.54
5	T	46	SEP	P-O3P	-2.08	1.47	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	46	SEP	O3P-P-O1P	3.01	122.57	110.83
5	T	46	SEP	O3P-P-O1P	2.68	121.27	110.83
5	L	46	SEP	O3P-P-O1P	2.58	120.88	110.83
5	T	46	SEP	OG-CB-CA	-2.41	105.80	108.14
5	Y	46	SEP	O3P-P-O1P	2.36	120.02	110.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	46	SEP	C-CA-CB-OG
5	T	46	SEP	CB-OG-P-O1P
5	T	46	SEP	CB-OG-P-O2P
5	T	46	SEP	CB-OG-P-O3P
5	L	46	SEP	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	46	SEP	2	0
5	Y	46	SEP	4	0
5	S	46	SEP	1	0
5	L	46	SEP	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
6	SO4	C	947	-	4,4,4	0.33	0	6,6,6	0.23	0
6	SO4	C	846	-	4,4,4	0.36	0	6,6,6	0.29	0
6	SO4	A	946	-	4,4,4	0.38	0	6,6,6	0.71	0
6	SO4	G	646	-	4,4,4	0.39	0	6,6,6	0.11	0
6	SO4	A	599	-	4,4,4	0.41	0	6,6,6	0.14	0
6	SO4	G	647	-	4,4,4	0.36	0	6,6,6	0.20	0
6	SO4	C	346	-	4,4,4	0.41	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	947	SO4	1	0
6	A	946	SO4	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	E	16/16 (100%)	-1.55	0	100	100	49, 75, 90, 91	0
1	H	16/16 (100%)	-1.49	0	100	100	52, 78, 93, 111	0
2	B	16/16 (100%)	-1.52	0	100	100	54, 79, 95, 104	0
2	R	16/16 (100%)	-1.57	0	100	100	46, 77, 94, 94	0
3	A	322/332 (96%)	-1.39	0	100	100	34, 80, 119, 141	0
3	C	322/332 (96%)	-1.35	0	100	100	33, 86, 119, 135	0
3	G	322/332 (96%)	-1.44	0	100	100	28, 71, 107, 127	0
4	D	323/332 (97%)	-1.28	0	100	100	33, 90, 129, 148	0
5	L	86/88 (97%)	-1.32	0	100	100	43, 79, 102, 127	0
5	S	86/88 (97%)	-1.35	0	100	100	43, 74, 96, 109	0
5	T	86/88 (97%)	-1.28	0	100	100	54, 75, 96, 103	0
5	Y	86/88 (97%)	-1.41	0	100	100	54, 75, 89, 111	0
All	All	1697/1744 (97%)	-1.37	0	100	100	28, 79, 118, 148	0

There are no RSRZ outliers to report.

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

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
5	SEP	T	46	10/11	0.99	0.05	54,66,74,75	0
5	SEP	L	46	10/11	0.99	0.05	49,59,66,72	0
5	SEP	Y	46	10/11	0.99	0.04	61,66,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SEP	S	46	10/11	0.99	0.03	48,58,66,69	0

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
6	SO4	G	646	5/5	0.98	0.06	139,141,143,146	0
6	SO4	G	647	5/5	0.98	0.04	120,123,124,127	0
6	SO4	C	947	5/5	0.99	0.07	133,136,138,141	0
6	SO4	C	846	5/5	0.99	0.11	94,98,99,102	0
6	SO4	C	346	5/5	0.99	0.04	113,119,120,122	0
6	SO4	A	599	5/5	0.99	0.04	109,114,116,116	0
6	SO4	A	946	5/5	0.99	0.05	110,111,114,115	0
7	MG	D	754	1/1	0.99	0.06	74,74,74,74	0
7	MG	A	704	1/1	1.00	0.01	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.