



wwPDB X-ray Structure Validation Summary Report

Apr 1, 2014 – 11:45 PM EDT

PDB ID : 3OQO
Title : Ccpa-hpr-ser46p-syn cre
Authors : schumacher, M.A.; Sprehe, M.; Bartholomae, M.; Hillen, W.; Brennan, R.G.
Deposited on : 2010-09-03
Resolution : 2.97 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

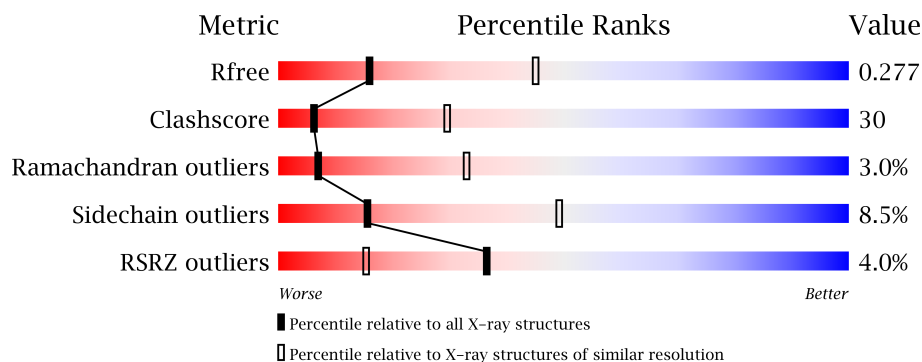
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.97 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}	66092	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	339	
1	C	339	
2	D	87	
2	S	87	
3	E	16	
4	B	16	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	399	-	X
5	SO4	A	499	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	C	599	-	X
5	SO4	C	699	-	X
5	SO4	C	999	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7160 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Catabolite control protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2584	1630	439	503	12			
1	C	332	Total	C	N	O	S	0	0	0
			2579	1627	438	502	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	EXPRESSION TAG	UNP P25144
A	336	HIS	-	EXPRESSION TAG	UNP P25144
A	337	HIS	-	EXPRESSION TAG	UNP P25144
A	338	HIS	-	EXPRESSION TAG	UNP P25144
A	339	HIS	-	EXPRESSION TAG	UNP P25144
A	340	HIS	-	EXPRESSION TAG	UNP P25144
C	335	HIS	-	EXPRESSION TAG	UNP P25144
C	336	HIS	-	EXPRESSION TAG	UNP P25144
C	337	HIS	-	EXPRESSION TAG	UNP P25144
C	338	HIS	-	EXPRESSION TAG	UNP P25144
C	339	HIS	-	EXPRESSION TAG	UNP P25144
C	340	HIS	-	EXPRESSION TAG	UNP P25144

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	S	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			
2	D	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			

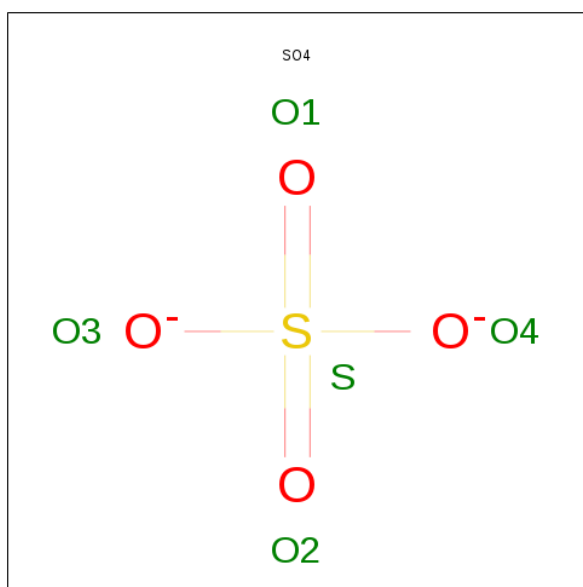
- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			

- Molecule 4 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
4	B	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



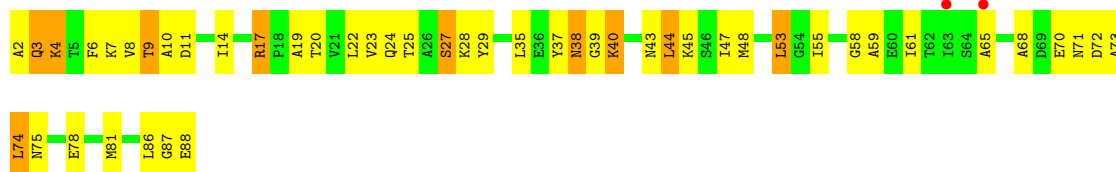
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total 23	O 23	0	0
6	S	8	Total 8	O 8	0	0
6	C	13	Total 13	O 13	0	0
6	E	2	Total 2	O 2	0	0
6	B	2	Total 2	O 2	0	0

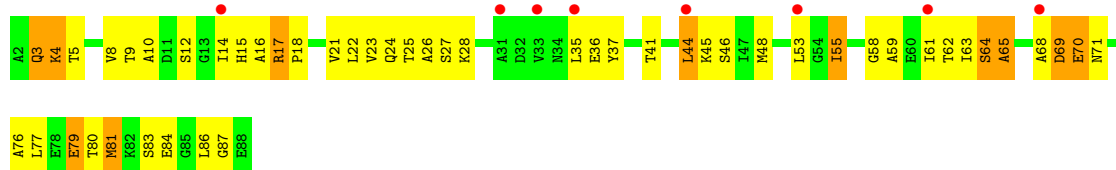
- Molecule 2: Phosphocarrier protein HPr

Chain S:



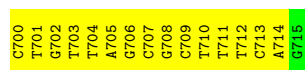
- Molecule 2: Phosphocarrier protein HPr

Chain D:



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

Chain E:



- Molecule 4: 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3',

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 105.21Å 173.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.40 – 2.97 56.40 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.0 (56.40-2.97) 99.0 (56.40-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.270 0.220 , 0.277	Depositor DCC
R_{free} test set	1959 reflections (6.87%)	DCC
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28497 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7160	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	A	0.39	0/2624	0.62	0/3556
1	C	0.36	0/2619	0.59	0/3549
2	D	0.33	0/630	0.52	0/846
2	S	0.36	0/630	0.55	0/846
3	E	0.57	0/360	0.79	0/554
4	B	0.58	0/368	0.80	0/566
All	All	0.39	0/7231	0.62	0/9917

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
4	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	700	DC	Sidechain
4	B	713	DC	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2584	0	2627	167	0
1	C	2579	0	2622	158	0
2	D	637	0	631	46	0
2	S	637	0	631	49	0
3	E	323	0	184	26	0
4	B	327	0	180	20	0
5	A	10	0	0	0	0
5	C	15	0	0	0	0
6	A	23	0	0	1	0
6	B	2	0	0	0	0
6	C	13	0	0	1	0
6	E	2	0	0	0	0
6	S	8	0	0	1	0
All	All	7160	0	6875	424	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

The worst 5 of 424 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:710:DT:H2''	3:E:711:DT:H5'	1.17	1.16
2:D:9:THR:HG22	2:D:87:GLY:H	1.16	1.10
1:A:30:VAL:HG23	1:A:35:ARG:HH21	1.11	1.09
1:C:89:MET:HG3	2:D:24:GLN:HE21	1.16	1.09
1:A:23:VAL:HG21	1:A:38:VAL:HG11	1.44	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	331/339 (98%)	281 (85%)	43 (13%)	7 (2%)	11	46
1	C	330/339 (97%)	279 (84%)	43 (13%)	8 (2%)	9	41
2	D	84/87 (97%)	64 (76%)	13 (16%)	7 (8%)	1	6
2	S	84/87 (97%)	70 (83%)	11 (13%)	3 (4%)	5	27
All	All	829/852 (97%)	694 (84%)	110 (13%)	25 (3%)	7	33

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	29	ASN
1	A	276	ASP
2	S	38	ASN
1	C	276	ASP

5.3.2 Protein sidechains ⓘ

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	286/292 (98%)	266 (93%)	20 (7%)	21	61
1	C	286/292 (98%)	263 (92%)	23 (8%)	17	52
2	D	66/66 (100%)	59 (89%)	7 (11%)	10	35
2	S	66/66 (100%)	56 (85%)	10 (15%)	4	18
All	All	704/716 (98%)	644 (92%)	60 (8%)	15	49

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	53	LEU
1	C	61	THR
2	D	17	ARG
1	C	11	ARG
1	C	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	S	24	GLN
1	C	102	ASN
2	D	15	HIS
1	C	98	ASN
1	C	101	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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, 95th 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	333/339 (98%)	0.08	10 (3%) 48 19	48, 74, 107, 142	0
1	C	332/339 (97%)	0.09	15 (4%) 32 14	46, 87, 124, 142	0
2	D	87/87 (100%)	0.21	8 (9%) 9 4	71, 114, 132, 142	0
2	S	87/87 (100%)	0.02	2 (2%) 57 23	58, 88, 111, 124	0
3	E	16/16 (100%)	-0.44	0 100 100	66, 81, 99, 100	0
4	B	16/16 (100%)	-0.35	0 100 100	66, 79, 98, 99	0
All	All	871/884 (98%)	0.07	35 (4%) 36 15	46, 83, 123, 142	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	MET	8.4
1	A	264	LEU	3.7
2	D	68	ALA	3.5
2	D	35	LEU	3.5
2	D	33	VAL	3.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SEP	D	46	10/11	0.15	-0.82	88,93,97,99	0
2	SEP	S	46	10/11	0.12	-0.98	51,62,65,71	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	C	699	5/5	0.31	11.86	165,166,167,168	0
5	SO4	A	399	5/5	0.20	4.76	131,135,138,138	0
5	SO4	A	499	5/5	0.22	4.49	126,127,132,133	0
5	SO4	C	999	5/5	0.33	3.93	177,178,178,178	0
5	SO4	C	599	5/5	0.25	3.57	152,152,154,155	0

6.5 Other polymers ⓘ

There are no such residues in this entry.